

The Periodic Table in Flatland

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Abstract

The D -dimensional Coulomb system serves as a starting point for generating generalized atomic shells. These shells are ordered according to a generalized Madelung rule in D dimensions. This rule together with an *Aufbau Prinzip* is applied to produce a D -dimensional periodic table. A model is developed to rationalize the ordering of the shells predicted by the generalized Madelung rule. This model is based on the introduction of an Hamiltonian, invariant under the q -deformed algebra $U_q(\mathfrak{so}(D))$, that breaks down the $\mathrm{SO}(D+1)$ dynamical symmetry of the hydrogen atom in D dimensions. The $D = 2$ case (Flatland) is investigated with some details. It is shown that the neutral atoms and the (moderately) positive ions correspond to the values $q = 0.8$ and $q = 1$, respectively, of the deformation parameter q .

Key words: D -dimensional hydrogen atom, Madelung rules, periodic tables, Flatland, *Aufbau Prinzip*.

1 Introduction

There exists a huge number of articles and books devoted to the classification of the chemical elements in the ordinary space (with $D = 3$ spatial dimensions). A nonexhaustive list of works presenting quantitative achievements is provided by Refs. [1-26]. In recent years, the classification of molecules in $D = 3$ dimensions was also the subject of numerous studies (see Refs. [27-30] and references cited therein).

Group theoretical and Lie algebraic methods play an important role in the classification of atoms and molecules. Along this vein, the authors recently used the notion of q -deformed Lie algebra for the classification of neutral atoms and positive ions in $D = 3$ dimensions [26]. From the mathematical point of view, the approach in Ref. [26] may be extended in the case where D is arbitrary.

The aim of this paper is two-fold: (i) to attack the problem of the classification of chemical elements in a space-time with D spatial dimensions and (ii) to examine the special case where $D = 2$. Indeed, the idea of chemical elements in D dimensions is already present in the consideration of a D -dimensional hydrogen atom. During the last four decades, hydrogen-like systems in D dimensions were the subject of numerous investigations (see for example Refs. [31-39]). As a next step, the study of many-electron systems in D dimensions is appealing. In this connection, the formulation of the quantum-mechanical many-body problem in terms of hyperspherical coordinates is of considerable interest [40-45]. The special case $D = 2$ is of great importance because of the specificities that arise in this case. This explains why several works have been devoted to Flatland [46] as far as dynamical systems and chemical elements are concerned [47-50].

The paper is organized as follows. In Section 2, we derive in a compact way those aspects (energy and degeneracy) of the D -dimensional nonrelativistic Coulomb system that are essential for Sections 3 and 4. Section 3 deals with an extension of the Madelung rule and an *Aufbau Prinzip* in D dimensions. A model for the generalized D -dimensional Madelung rule is given in Section 4. The case of Flatland ($D = 2$) is discussed in Sections 3, 4, and 5.

2 The Hydrogen Atom in D Dimensions

2.1. The discrete spectrum

The Schrödinger equation for a D -dimensional hydrogen-like atom of nuclear charge Ze ($Ze > 0$) and reduced mass μ reads

$$-\frac{\hbar^2}{2\mu} \Delta \Psi + V \Psi = E \Psi, \quad (1)$$

where Δ is the Laplace operator and V the potential energy in D dimensions ($D \geq 2$).

We assume that

$$V = -\frac{Ze^2}{r}, \quad (2)$$

where r is the hyperradius. Note that for $D = 2$ and $D \geq 3$, the potential V should be taken in the form $V \sim Ze^2 \ln r$ and $V \sim -Ze^2 r^{2-D}$, respectively, if one imposes that V satisfies the Poisson equation (cf. Ref. [37]). Note also that the potential energy V could be chosen in the form (2) where Z exhibits a dependence on the hyperspherical angular coordinates $\Omega \equiv (\theta_1, \theta_2, \dots, \theta_{D-2}, \varphi)$ (see Refs. [41,42]); the latter choice is especially appropriate to take into account correlation effects in many-particle systems. In the present paper, we take V as given by (2) where Z is a constant for the sake of simplicity and in order to have an expression that generalizes in a simple manner the usual potential energy in $D = 3$ dimensions. In view of the applications to the construction of periodic tables, we are interested in the discrete eigenvalues of the energy E ($E < 0$) in Eq. (1). These eigenvalues can be found as follows.

Let us look for a solution of Eqs. (1-2) in the form

$$\Psi(r, \Omega) = R(r) Y_{[\ell]}(\Omega), \quad (3)$$

where $Y_{[\ell]}$ denotes an hyperspherical harmonic in D dimensions. This leads, after separation of variables, to the radial equation

$$-\frac{\hbar^2}{2\mu} \left[\frac{d^2 R}{dr^2} + \frac{D-1}{r} \frac{dR}{dr} - \frac{\ell(\ell+D-2)}{r^2} R \right] - \frac{Ze^2}{r} R = ER, \quad (4)$$

where $\ell(\ell+D-2)$, with $\ell \in \mathbb{N}$, is an eigenvalue of the square of the angular momentum in D dimensions (see also the book by Avery [45]). (In the $D = 2$ case, the orbital angular

momentum ℓ is simply $|m_\ell|$.) By putting

$$\rho = 2\alpha r, \quad \alpha = \frac{\sqrt{-2\mu E}}{\hbar}, \quad k = \frac{\mu Ze^2}{\alpha\hbar^2}, \quad \nu = \ell + \frac{1}{2}(D-2) \quad (5)$$

and by making the change of function

$$R(r) = \rho^{-(D-1)/2} W(\rho), \quad (6)$$

Eq. (4) can be transformed into the Whittaker differential equation [51]:

$$W'' + \left(-\frac{1}{4} + \frac{k}{\rho} + \frac{\frac{1}{4} - \nu^2}{\rho^2} \right) W = 0. \quad (7)$$

By retaining only the solutions regular at the origin of Eq. (7), we obtain the total wave function

$$\Psi(r, \Omega) = (2\alpha r)^\ell e^{-\alpha r} {}_1F_1\left(\frac{1}{2} - k + \nu, 2\nu + 1; 2\alpha r\right) Y_{[\ell]}(\Omega), \quad (8a)$$

where ${}_1F_1$ is the confluent hypergeometric function.

The discrete eigenvalues for the energy E are obtained by requiring that the total wave function Ψ belongs to $L^2(\mathbb{R}^D)$. This yields the quantization condition

$$\frac{1}{2} - k + \nu = -n_r, \quad n_r \in \mathbb{N}, \quad (9)$$

where n_r is referred to as the radial quantum number. By combining Eqs. (5) and (9), we obtain that the discrete energy spectrum is given by (cf. Refs. [31,32,36,38])

$$E = \frac{E_0}{[N + \frac{1}{2}(D-1)]^2}, \quad E_0 = -\frac{\mu(Ze^2)^2}{2\hbar^2}, \quad N = n_r + \ell, \quad N \in \mathbb{N}. \quad (10)$$

The possible values of ℓ are $\ell = 0, 1, \dots, N$. (Observe that for $D = 3$, we have $N = n - 1$, where n is the usual principal quantum number. Note also that Eq. (10) can be applied to $D = 1$ under the condition to omit the state for which $N = 0$.) Equation (10) can be transformed to yield

$$E = \frac{E_0}{\Lambda^2 + (\frac{D-1}{2})^2}, \quad \Lambda^2 = \lambda(\lambda + D - 1), \quad \lambda = n_r + \ell, \quad (11)$$

an expression which constitutes a starting point for the developments in Section 4. The quantity Λ^2 in Eq. (11) turns out to be an eigenvalue of the second-order Casimir operator

of the special orthogonal group $\text{SO}(D + 1)$ in $D + 1$ dimensions. In other words, $\Lambda^2 \equiv \lambda(\lambda + D + 1 - 2)$, with $\lambda \in \mathbb{N}$, is an eigenvalue of the square of the angular momentum in $D + 1$ dimensions. Equation (11) is the transcription in terms of eigenvalues of the connection between the hydrogen-like atom in D dimensions and the symmetrical spherical rotor in $D + 1$ dimensions. Moreover, the energy formula (11) reflects the $\text{SO}(D + 1)$ dynamical symmetry of the Coulomb system in D dimensions. This is reminiscent of the application of the Fock stereographic projection to the hydrogen atom in D dimensions (projection of \mathbb{R}^D onto the unit sphere of \mathbb{R}^{D+1}). As a point of fact, by applying the Fock transformation [52] to the D -dimensional Schrödinger equation (in momentum space) for the hydrogen-like atom, we get [31,32,45]

$$\frac{1}{\sqrt{-2\mu E}} \frac{\mu Z e^2}{\hbar} = \lambda + \frac{1}{2} (D - 1), \quad \lambda \in \mathbb{N}, \quad (12)$$

which leads to Eq. (11).

Finally, by using Eq. (9) the wave function (8a) becomes

$$\Psi(r, \Omega) = N_{N,\ell} (2\alpha r)^\ell e^{-\alpha r} {}_1F_1\left(-n_r, 2\nu + 1; 2\alpha r\right) Y_{[\ell]}(\Omega), \quad (8b)$$

where the normalization constant $N_{N,\ell}$ is

$$N_{N,\ell} = \frac{1}{(2\ell + D - 2)!} \left[\frac{(2\alpha)^D (N + \ell + D - 2)!}{(2N + D - 1) (N - \ell)!} \right]^{1/2}, \quad (13)$$

up to an arbitrary phase factor. Equations (8b) and (13) are in agreement with the results in Ref. [42]. Following the usual terminology used in the $D = 3$ case, we shall refer the wave function (8b) as an atomic orbital. The various atomic orbitals corresponding to given values of $N + 1$ and ℓ define a shell denoted as $(N + 1, \ell)$. As for the $D = 3$ case, we shall use the notation $\ell = \text{s, p, d, } \dots$ instead of $\ell = 0, 1, 2, \dots$ for the angular momentum in $(N + 1, \ell)$.

2.2. Degeneracies of the spectrum

The dimension of the subspace spanned by the angular wave functions $Y_{[\ell]}(\Omega)$ corresponding to a given value of ℓ is

$$g(\ell, D) = \frac{(2\ell + D - 2) (\ell + D - 3)!}{\ell! (D - 2)!}, \quad D \geq 3 \quad (14a)$$

that is nothing but the dimension of the irreducible representation $[\ell, 0, 0, \dots, 0]$ (with $D - 2$ entries) of the geometrical symmetry group $\text{SO}(D)$ of the hydrogen-like atom in D dimensions. Indeed, $g(\ell, D)$ corresponds to the essential (i.e., geometrical or orbital) degeneracy of the energy level E given by Eq. (10). The dimension formula (14a) can be simply obtained [34] (see also [33,45]) as the difference between the dimension of the space of the homogeneous polynomials with degree ℓ in \mathbb{R}^D and the dimension of the space of the homogeneous polynomials with degree $\ell - 2$ in \mathbb{R}^D (arising from the action of the generalized Laplace operator on the homogeneous polynomials with degree ℓ in \mathbb{R}^D). As an example, Eq. (14a) with $D = 3$ gives back the well-known result $g(\ell, 3) = 2\ell + 1$. For $D = 2$, note that Eq. (14a) gives $g(\ell, 2) = 2$ for $\ell \neq 0$ and is not valid for $\ell = 0$. (In fact, we have $g(0, 2) = 1$ that follows from $g(0, D) = 1$.) Returning to the case where D is arbitrary, we note that

$$g(\ell, D) = g(\ell, D - 1) + g(\ell - 1, D) \quad (14b)$$

so that $g(\ell, D)$ can be obtained in an iterative fashion from $g(0, D) = 1$ and $g(\ell, 2) = 2 - \delta(\ell, 0)$.

We are now in a position to simply obtain the degree of degeneracy of the energy level E given by Eqs. (10-11). It is mentioned above that Eq. (11) for E shows that the hydrogen-like atom in D dimensions is connected to the symmetrical spherical rotor in $D + 1$ dimensions. Consequently, the degree of degeneracy of E is equal to the degree of degeneracy of the eigenvalue $\lambda(\lambda + D + 1 - 2)$ of the second-order invariant of $\text{SO}(D + 1)$. The latter degree of degeneracy is given by Eq. (14a) with $\ell \mapsto N$ and $D \mapsto D + 1$ since the relevant special orthogonal group is $\text{SO}(D + 1)$ and $\lambda = N = n_r + \ell$. As a conclusion, the total degree of degeneracy g (covering essential and accidental degeneracies) of the energy level E given by Eq. (10) is

$$g \equiv g(N, D + 1) = \frac{(2N + D - 1)(N + D - 2)!}{N!(D - 1)!}, \quad N \in \mathbb{N}. \quad (15)$$

The expression in the second right-hand side of Eq. (15) is a well-known result. (See for instance Ref. [45] where this expression is derived from the theory of hyperspherical harmonics.) The significance of Eq. (15) is clear: for $N + 1$ fixed, the g orbitals (8b) with

$\ell = 0, 1, \dots, N$ have the energy (10). By way of illustration, we have $g = 2N + 1$ for $D = 2$ and $g = (N + 1)^2 = (n_r + \ell + 1)^2 = n^2$ for $D = 3$. We thus recover the Stoner number $g = n^2$ for the ordinary hydrogen atom.

3 Madelung Rule and Aufbau Prinzip

We now examine the problem of the distribution of the Z electrons of a neutral atom on the generalized atomic orbitals. Such a distribution does not make sense if the energy of the shell $(N + 1, \ell)$ is given by Eqs. (10-11) since the energy formula (10) does not take into account the interelectronic repulsion between the Z electrons of a complex atom. We shall introduce in Section 4 a symmetry breaking mechanism in order to generate monoelectronic energy levels depending on $N + 1$ and ℓ . We thus continue with the filling of the Z electrons on atomic shells $(N + 1, \ell)$ that do not present anymore accidental degeneracies.

In the ordinary case ($D = 3$), it is a well-known fact that the filling of the shells $(N + 1, \ell)$, with $N + 1 = n$, according to the rule – n increasing and, for n fixed, to ℓ increasing – does not correspond to a realistic situation for $Z \geq 19$ (see Ref. [1]). In the $D = 2$ case, it has been shown [50], on the basis of Hartree-Fock calculations, that this rule ($N + 1$ increasing and, for $N + 1$ fixed, $\ell = |m_\ell|$ increasing) stops working for $Z \geq 15$: for $Z = 15$, the energy of the shell (4,s) is lower than the one of the shell (3,d). In both cases, an alternative rule for the filling of the shells has to be found. When $D = 3$, such a rule is known as the Madelung (or Madelung-Klechkovskii, or Madelung-Goudsmit-Bose) rule [2-5]. (In the $D = 3$ case, this rule was implicit in the 1922 Bohr *Aufbau Prinzip* [1] and was set out in 1926 by Madelung [4].) We shall formulate this rule in the case where D is arbitrary ($D \geq 2$) and we shall apply it to the particular cases $D = 2$ and 3.

The generalized Madelung rule can be expressed in the following way. The electronic shells $(N + 1, \ell)$ are filled according to: (i) $N + 1 + \ell$ increasing and (ii) $N + 1$ increasing for $N + 1 + \ell$ fixed. The obtained filling can be described by the following sequence of shells

$$(1, s) < (2, s) < (2, p) < (3, s) < (3, p) < (4, s) < (3, d) < (4, p) < (5, s) <$$

$$(4, d) < (5, p) < (6, s) < (4, f) < (5, d) < (6, p) < (7, s) < (5, f) < (6, d) < (7, p) < \dots \quad (16)$$

The ordering (16) is identical to the one predicted by the usual Madelung rule corresponding to $D = 3$.

We are now prepared for describing an *Aufbau Prinzip* in D dimensions. Each $(N+1, \ell)$ shell in (16) can be filled with $2g(\ell, D)$ electrons, where $g(\ell, D)$ is given by (14a), the factor 2 coming from the fact that each orbital gives rise to two spin-orbitals. [As for $D = 3$, we admit that the spectral group that labels the spin is $SU(2)$ and that the Pauli principle works.] The generalized Madelung rule can be depicted by the diagram

$$\begin{array}{c} [1, 1] \\ [2, 2] [3, 2] \\ [3, 3] [4, 3] [5, 3] \\ [4, 4] [5, 4] [6, 4] [7, 4] \\ [5, 5] [6, 5] [7, 5] [8, 5] [9, 5] \dots \\ \dots \end{array} \quad (17)$$

In (17) the rows are labelled with $N+1 = 1, 2, 3, \dots$ and the columns with $\ell = 0, 1, 2, \dots$ and the entry at the intersection of the $(N+1)$ th row and ℓ th column is denoted as $[N+1+\ell, N+1]$ (with, for fixed $N+1$, $\ell = 0, 1, \dots, N$). This diagram provides us with the skeleton of a periodic table where the places for the various “chemical elements” are obtained by replacing each entry $[N+1+\ell, N+1]$ of the diagram by a block $\{\dots\}$. Each block corresponds to given values of $N+1$ and ℓ . The block $\{\dots\}$ associated to the entry $[N+1+\ell, N+1]$ of the diagram contains $2g(\ell, D)$ elements.

In the $D = 3$ case, this *Aufbau Prinzip* leads to the periodic table [23]

$$\begin{array}{l} \{001, 002\} \\ \{003, 004\} \{005, 006, \dots, 010\} \\ \{011, 012\} \{013, 014, \dots, 018\} \{021, 022, \dots, 030\} \\ \{019, 020\} \{031, 032, \dots, 036\} \{039, 040, \dots, 048\} \{057, 058, \dots, 070\} \\ \{037, 038\} \{049, 050, \dots, 054\} \{071, 072, \dots, 080\} \{089, 090, \dots, 102\} \{\dots \\ \{055, 056\} \{081, 082, \dots, 086\} \{103, 104, \dots, 112\} \{\dots \\ \{087, 088\} \{113, 114, \dots, 118\} \{\dots \\ \{119, 120\} \{\dots \\ \{\dots \end{array} \quad (18)$$

Each neutral atom in (18) is characterized by its atomic number Z ($001 \equiv 1$, $002 \equiv 2$, $003 \equiv 3$, \dots). In the table (18), the various periods of the Mendeleev table are identified by reading the table in the dictionary order, as in the diagram (17), and by stopping at the end of a $(N+1, p)$ shell (except for the first period). It is to be reminded that the table (18) can be rationalized through the use of the group $SO(4, 2) \otimes SU(2)$. (For more details, see Refs. [10,12,16,23].)

In the $D = 2$ case, the generalized Madelung rule gives also the ordering described by the sequence (16) with $(N+1, \ell) \equiv (N+1, |m_\ell|)$. The filling, with two $[2g(0, 2) = 2]$ electrons in each $(N+1, s)$ shell and four $[2g(\ell \neq 0, 2) = 4]$ electrons in each $(N+1, \ell \neq s)$ shell, of the sequence (16) corresponds to the following periods with their degeneracies (the degeneracy of a period is the number of elements in the period)

$$\begin{aligned}
& (1, s) : 2 \\
& (2, s) (2, p) : 6 \\
& (3, s) (3, p) : 6 \\
& (4, s) (3, d) (4, p) : 10 \\
& (5, s) (4, d) (5, p) : 10 \\
& (6, s) (4, f) (5, d) (6, p) : 14 \\
& (7, s) (5, f) (6, d) (7, p) : 14 \\
& \dots
\end{aligned} \tag{19}$$

The set of periods (19) reflects (like in the $D = 3$ case) a period doubling, except for the first period. The diagram (17) then leads to the following periodic table

$$\begin{aligned}
& \{001, 002\} \\
& \{003, 004\} \{005, 006, 007, 008\} \\
& \{009, 010\} \{011, 012, 013, 014\} \{017, 018, 019, 020\} \\
& \{015, 016\} \{021, 022, 023, 024\} \{027, 028, 029, 030\} \{037, 038, 039, 040\} \\
& \{025, 026\} \{031, 032, 033, 034\} \{041, 042, 043, 044\} \{051, 052, 053, 054\} \{\dots \\
& \{035, 036\} \{045, 046, 047, 048\} \{055, 056, 057, 058\} \{\dots \\
& \{049, 050\} \{059, 060, 061, 062\} \{\dots \\
& \{063, 064\} \{\dots \\
& \{\dots
\end{aligned} \tag{20}$$

Here again, the “chemical elements” in the blocks of (20) are characterized by their atomic number Z . Furthermore, the elements in a given block (corresponding to $[N+1+\ell, N+1]$)

can be distinguished by two heuristic quantum numbers, namely, $m_\ell = \mp \ell$ and $\sigma = \mp 1/2$. Then, the address Z of an element in the block attached to $[N+1, \ell]$ is given by

$$Z(N+1, \ell, m_\ell, \sigma) = (N+1+\ell)^2 - \frac{1}{2} \left[1 + (-1)^{N+1+\ell} \right] - 2 \left[2\ell + \delta(\ell + m_\ell, 0) - 1 \right] + \sigma + \frac{1}{2}, \quad (21)$$

with $N+1 = 1, 2, 3, \dots$; $\ell = 0, 1, \dots, N$; $m_\ell = \mp \ell$; and $\sigma = \mp 1/2$. For instance, $Z = 11$ corresponds to $N+1 = 3$, $\ell = 1$, $m_\ell = -1$, and $\sigma = -1/2$ while $Z = 40$ corresponds to $N+1 = 4$, $\ell = 3$, $m_\ell = +3$, and $\sigma = +1/2$. In the block corresponding to $[N+1+\ell, N+1]$, the number Z increases with m_ℓ (m_ℓ passing from $-\ell$ to $+\ell$) and, for m_ℓ fixed, with σ (σ passing from $-1/2$ to $+1/2$).

As for the $D = 3$ case [17,20], it is possible to define a key function for $D = 2$. The key function Z_ℓ is the atomic number Z for which (at least) one electron with angular momentum ℓ appears for the first time. (Note that this definition works for D arbitrary too.) By adapting to the $D = 2$ case the derivation by Essén [20], the key function reads

$$Z_\ell = 2 \left[\sum_{N=0}^{\ell-1} 2g(N, 3) \right] + 1 = 2 \left[\sum_{N=0}^{\ell-1} 2(2N+1) \right] + 1, \quad \text{for } \ell \geq 1, \quad (22)$$

where the first factor 2 refers to the “double shell” structure (that manifests itself in a diagram connecting the hydrogen-like and Madelung orderings, see Ref. [20]) and the second to the spin. (Note that $Z_0 = 1$.) A simple calculation gives

$$Z_\ell = 4\ell^2 + 1. \quad (23)$$

For example, we have $Z_\ell = 1, 5, 17$, and 37 for the first appearance of the s, p, d, and f electrons, respectively, as can be checked from (20).

4 A Model for the Madelung Rule in Flatland

As already mentioned at the beginning of Section 3, the derivation of a model for justifying the Madelung rule in D dimensions cannot be carried out with the help of the energy formula (11). Following Novaro et al. [9,11,13,14] and Négadi and Kibler [26], a possible way to find an energy formula that reproduces the generalized Madelung rule is to introduce, in the context of q -deformations, an anisotropic term in the denominator of Eq. (11). This can be done by replacing in (11) the eigenvalue $\Lambda^2 \equiv \Lambda_{D+1}^2$ of the Casimir

of the group $\text{SO}(D+1)$ by $\Lambda_{D+1}^2 + \alpha(q)\Lambda_D^2(q)$, where $\Lambda_D^2(q)$ stands for an invariant operator of the q -deformed algebra $U_q(\text{so}(D))$ and $\alpha(q)$ denotes a constant depending on the deformation parameter q . (See Refs. [53-55] for an introduction to q -deformed – or quantum – algebras.) To be more precise, the formula (11) is replaced by

$$E = \frac{E_0}{\Lambda_{D+1}^2 + \alpha(q)\Lambda_D^2(q) + (\frac{D-1}{2})^2} = \frac{E_0}{(N + \frac{D-1}{2})^2 + \alpha(q)\Lambda_D^2(q)}. \quad (24)$$

In terms of symmetries, the dynamical symmetry $\text{SO}(D+1)$ is replaced by the symmetry $\text{SO}(D+1) \supset U_q(\text{so}(D))$, where the quantum algebra $U_q(\text{so}(D))$ describes a symmetry breaking mechanism.

In the $D = 3$ case, the formula (24) was applied in Ref. [26] with

$$\Lambda_4^2 = (N+1)^2 - 1 = n^2 - 1, \quad \Lambda_3^2(q) = [\ell]_q[\ell+1]_q, \quad \alpha(q) = 3 - \frac{5}{3}q, \quad (25)$$

where the (q -deformed) quantities of type $[x]_q$ are defined by

$$[x]_q = \frac{q^x - q^{-x}}{q - q^{-1}}. \quad (26)$$

The situation where $q = 1$ gives back the Novaro [14] model for neutral atoms [corresponding to the ordering (16)]. Furthermore, it was shown [26] that Eq. (24) with $D = 3$ furnishes a model that describes neutral atoms for $q = 0.9$ [with the ordering (16)] and positive ions for $1.15 \leq q \leq 1.30$ [with an ordering different from (16)].

We now focus our attention on the $D = 2$ case. In this case, the dynamical symmetry $\text{SO}(3)$ has to be replaced by the symmetry $\text{SO}(3) \supset \text{SO}(2)$ since the one-parameter Lie algebra $\text{so}(2)$ cannot be deformed. We can however consider a q -deformation of the eigenvalue $\ell = |m_\ell|$ in order to mimick the approach followed in Ref. [26] for the $D = 3$ case. Therefore we particularize, to the $D = 2$ case, Eq. (24) in the form

$$E = \frac{E_0}{N(N+1) + \alpha(q)([\ell]_q)^2 + \frac{1}{4}}, \quad (27)$$

where the anisotropy parameter $\alpha(q)$ is taken to be

$$\alpha(q) = 3 - \frac{5}{3}q, \quad (28)$$

as for the $D = 3$ case [26]. Then, Eq. (27) becomes

$$E = \frac{E_0}{(N + \frac{1}{2})^2 + (3 - \frac{5}{3}q)([\ell]_q)^2}, \quad (29)$$

where the q -deformed number $[\ell]_q$ can be developed as

$$[\ell]_q = q^{\ell-1} + q^{\ell-3} + \cdots + q^{-\ell+1} \quad \text{for } \ell \neq 0, \quad (30)$$

an expression which may be prolonged by $[0]_q = 0$. In order to find the ordering of the shells $(N+1, \ell)$ afforded by the energy formula (29), it is sufficient to consider the dimensionless quantity

$$\epsilon(N+1, \ell) = \sqrt{\left(N + \frac{1}{2}\right)^2 + \left(3 - \frac{5}{3}q\right)([\ell]_q)^2} \quad \text{with } N \in \mathbb{N} \text{ and } \ell = 0, 1, \dots, N \quad (31)$$

that gives the energy position of the shell $(N+1, \ell)$.

We have done an optimization of Eq. (31). As a result, for $q = 0.8$ we find, with a reasonable precision, that the energies given by Eq. (29) reproduce the ordering (16). The model inherent to Eq. (29) is thus in agreement with the two-dimensional Madelung rule especially for the lower shells. For instance, we have (for $q = 0.8$) the sequence

$$\begin{aligned} \epsilon(1, s) = 0.5 < \epsilon(2, s) = 1.5 < \epsilon(2, p) = 2.0 < \epsilon(3, s) = 2.5 < \\ \epsilon(3, p) = 2.8 < \epsilon(4, s) = 3.5 < \epsilon(3, d) = 3.6 < \epsilon(4, p) = 3.7 \end{aligned} \quad (32)$$

corresponding to Z varying from 1 to 24. The ordering (32) is the same as the one found by Pyykkö and Zhao [50] from Hartree-Fock calculations using a Gaussian basis and assuming $1/r$ Coulomb interactions. We note that the fitting value $q = 0.8$ is of the same magnitude as the value $q = 0.9$ obtained in the $D = 3$ case [26].

In the situation where $q = 1$, Eq. (29) leads to the following ordering

$$\begin{aligned} (1, s) < (2, s) < (2, p) < (3, s) < (3, p) < (3, d) < (4, s) < (4, p) < (4, d) < \\ (5, s) < (5, p) < (4, f) < (5, d) < (6, s) < (6, p) < (5, f) < (6, d) < (7, s) < \cdots \end{aligned} \quad (33)$$

which is identical to the ordering for the positive ions in the $D = 3$ case [18,19,26]. Unfortunately, there does not exist data (of Hartree-Fock type for example) for the positive ions in the $D = 2$ case. Therefore, the sequence (33) should be considered as a prediction for positive ions in two dimensions. To be more precise, the passage from $q = 0.8$ to $q = 1$ for $D = 2$ corresponds to the passage from neutral atoms to moderately ionized atoms,

a situation that parallels the one for $D = 3$ where q goes from 0.9 (neutral atoms) to 1.15 (positive ions) [26]. In the $D = 2$ case, we can expect that the highly ionized atoms correspond to increasing values of q since the limiting case of a hydrogen-like atom (for which the energy E increases with $N + 1$) is reached for $q = 1.8$ [see Eq. (29)].

5 Closing Remarks

In the present paper, we concentrated on three points: (i) the extension of the Madelung rule in D dimensions, (ii) an algorithm (*Aufbau Prinzip*) for constructing a periodic table in D dimensions, and (iii) a model for reproducing the ordering of the atomic shells in D dimensions. For each point, a special emphasis was put on the $D = 2$ case.

The periodic table for $D = 2$, obtained by means of the Madelung rule, resembles the one worked out in Ref. [23] except that the blocks contain two or four elements. We gave an address formula [Eq. (21)] for locating the element with atomic number Z in the periodic table. In addition, the key function for the first appearance of an electron of type ℓ in the periodic table was found to be $Z_\ell = 4\ell^2 + 1$. This key function compares with $Z_\ell = 2\ell^2 + 1$ that can be deduced from the work by Asturias and Aragón [47], where the Coulomb potential is taken in a logarithmic form. (Note that the “double shell” structure mentioned in Section 3 does not appear when the potential is logarithmic.)

The model developed in Section 4 on the basis of Eq. (24) relies on the connection between the hydrogen atom in D dimensions and the spherical rotor in $D + 1$ dimensions. Two important ingredients were used in conjunction with the latter connection, viz, the introduction of an anisotropic term as in the Novaro [14] model for $D = 3$ and the introduction of a q -deformation as in the Négadi-Kibler [26] model for $D = 3$. The model set up for D arbitrary was applied to $D = 2$ and it was shown that the deformation parameter q can discriminate between neutral atoms ($q = 0.8$) and positive ions ($q = 1$).

If we take the same notations for the chemical elements in two dimensions as the ones

employed in Ref. [50], the periodic table (20) takes the form

$$\begin{array}{ccccccc}
\{\text{H}^1 & \text{He}^2\} & & & & & \\
\{\text{Li}^3 & \text{Be}^4\} & & \{\text{B}^5 & \text{N}^6 & \text{F}^7 & \text{Ne}^8\} \\
\{\text{Na}^9 & \text{Mg}^{10}\} & & \{\text{Al}^{11} & \text{P}^{12} & \text{Cl}^{13} & \text{Ar}^{14}\} & & \{\text{Sc}^{17} & \text{Mg}^{18} & \text{Cu}^{19} & \text{Zn}^{20}\} \\
\{\text{K}^{15} & \text{Ca}^{16}\} & & \{\text{Ga}^{21} & \text{As}^{22} & \text{Br}^{23} & \text{Kr}^{24}\} & & & & &
\end{array} \tag{34}$$

if we restrict ourselves to $1 \leq Z \leq 24$. (The address Z for each element is indicated as a right upper subscript.) The table (34) is similar to the table in Ref. [50]: the two tables exhibit the same blocks in different arrangements. The main difference between the two tables is the position of the *transition metals* (Sc, Mn, Cu, Zn). The atomic configurations arising from the latter table are in accordance with those derived by Pyykkö and Zhao [50] from self-consistent field calculations, except for the “Scandium” ($Z = 17$). Indeed, according to our periodic table, the element Sc has the configuration $[\text{Ar}]4s^23d$, a fact to be contrasted with the configuration $[\text{Ar}]4s3d^2$ obtained in Ref. [50].

To close this paper, we would like to mention that the developments in the present work could be considered as a first step towards a classification of molecules in two dimensions. We hope to return on this subject in the future.

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